

The pseudogap Fermi-Bose Kondo model

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We consider a magnetic impurity coupled to both fermionic quasiparticles with a pseudogap density of states and bosonic spin fluctuations. Using renormalization group and large- N calculations we investigate the phase diagram of the resulting Fermi-Bose Kondo model. We show that the Kondo temperature is strongly reduced by low-energy spin fluctuations, and make connections to experiments in cuprate superconductors. Furthermore we derive an *exact* exponent for the critical behavior of the conduction electron T matrix, and propose our findings to be relevant for certain scenarios of local quantum criticality in heavy-fermion metals.

The interplay of quasiparticles and collective low-energy excitations is a central theme in the physics of strongly correlated materials. Impurities have proven to be a powerful probe for investigating the bulk behavior of such systems. A paradigmatic model describing the interaction of impurity degrees of freedom with both quasiparticles and collective spin fluctuations is the so-called Fermi-Bose Kondo model [1, 2], consisting of a local impurity spin, \vec{S} , coupled to spin- $\frac{1}{2}$ fermions and spin-1 vector bosons.

The Fermi-Bose Kondo model has recently been analyzed for the case of a metallic fermion density of states (DOS), and a gapless bosonic spectrum representing magnetic order parameter fluctuations at a bulk quantum critical point in d dimensions [1, 2]. For $d < 3$ the model shows a boundary quantum phase transition between a Kondo-screened phase and a bosonic fluctuating phase with universal local spin correlations. Both the critical and the bosonic fluctuating fixed points are characterized by singular thermodynamic properties, connected with local non-Fermi liquid behavior.

The purpose of this Letter is to generalize this analysis to a fermionic bath with a pseudogap DOS, $\rho_c(\omega) \propto |\omega|^r$, and to discuss Kondo screening for the case of a finite spin gap, Δ_s , in the bosonic bath. Using renormalization group (RG) methods, we shall establish the phase diagram of the pseudogap Fermi-Bose Kondo model, and furthermore derive an exact relation between the anomalous exponent of the fermion T matrix and the exponent of fermionic bath DOS, r , which holds at any fixed point with a finite coupling between fermions and impurity spin. We shall apply our model to impurity moments in cuprate superconductors, where the fermionic DOS obeys $r = 1$, and show that Kondo screening is strongly suppressed by collective spin fluctuations, in agreement with NMR experiments.

Recently, the Fermi-Bose Kondo model has been proposed [3] to describe a “local quantum phase transition” in alloys like $\text{CeCu}_{6-x}\text{Au}_x$ [4]. This modelling is based on an extended dynamical mean-field theory [3], where a lattice model is mapped onto a self-consistent single-impurity model. Based on our T matrix analysis, we will argue that no anomalous power law can occur in the

fermion spectrum within such a scenario of local criticality.

Model. The Fermi-Bose Kondo Hamiltonian for a spin- $\frac{1}{2}$ impurity can be written as $H = H_f + H_b + H_{\text{imp}}$, with

$$H_{\text{imp}} = J_K \vec{S} \cdot \vec{s}_0 + \gamma_0 \vec{S} \cdot \vec{\phi}_0. \quad (1)$$

Here, \vec{S} denotes the impurity spin operator, and H_f describes a system of free fermions, $H_f = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$ in standard notation, $\vec{s}_0 = \sum_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\sigma}^\dagger \vec{\sigma}_{\sigma\sigma'} c_{\mathbf{k}'\sigma'}$ is the conduction band spin operator at the impurity site $\mathbf{r}_0 = 0$. The fermionic density of states follows a power law at low energies, $\rho_c(\omega) = \sum_{\mathbf{k}} \delta(\omega - \epsilon_{\mathbf{k}}) \propto N_0 |\omega|^r$, which includes the cases of a metal ($r=0$) and a d -wave superconductor ($r=1$). In the simplest case, the bosonic bath consists of free vector bosons, $H_b = \sum_{\mathbf{q}\alpha} \omega_{\mathbf{q}} b_{\mathbf{q}\alpha}^\dagger b_{\mathbf{q}\alpha}$, describing collective spin fluctuations in the host material, with a dispersion $\omega_{\mathbf{q}}^2 = m^2 + c^2 \mathbf{q}^2$. At zero temperature, the mass m coincides with the bulk spin gap Δ_s . A gap $\Delta_s > 0$ describes a quantum paramagnet, $\Delta_s = 0$ corresponds to a bulk quantum critical point between the paramagnet and an antiferromagnetically ordered phase; the momentum \mathbf{q} is measured relative to the ordering wavevector \mathbf{Q} . The field $\vec{\phi}_0$ in Eq. (1) represents the local orientation of the antiferromagnetic order parameter, it is given by $\phi_{0\alpha} = \sum_{\mathbf{q}} (b_{\mathbf{q}\alpha} + b_{-\mathbf{q}\alpha}^\dagger) / \sqrt{\omega_{\mathbf{q}} J}$, where J is the bulk exchange constant. It is useful to define a spectral density, $\rho_\phi(\omega)$, of the Bose field ϕ . At $T = 0$ and for $\Delta_s = 0$, it follows $\rho_\phi(\omega) \propto K_0^2 \text{sgn}(\omega) |\omega|^{1-\epsilon}$, $K_0^2 = J/c^d$, in $d=3-\epsilon$ dimensions. We note that in dimensions $d < 3$, boson self-interactions are relevant in the RG sense (in the absence of Landau damping), and we will comment on their effect below. Our analysis will be restricted to the SU(2)-invariant model; the effect of spin anisotropy for $r=0$ has been discussed in Ref. 2.

In the absence of the bosonic bath, $\gamma=0$, and for $r=0$ the model (1) reduces to the well-known Kondo model [5], which exhibits screening of the magnetic moment below a characteristic (Kondo) temperature, T_K . The pseudogap generalization, $r > 0$, shows a zero-temperature phase transition between a free local moment and a screened moment as the Kondo coupling is varied [6, 7, 8, 9]. On the other hand, in the absence of the fermionic bath,

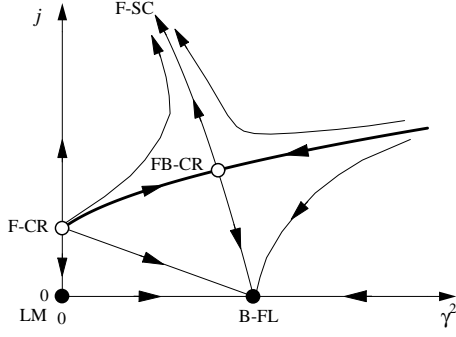


FIG. 1: Schematic RG flow diagram for the pseudogap Fermi-Bose Kondo model for small ϵ and r , and $\Delta_s = 0$. The axes denote the couplings to the bosonic (γ) and fermionic (j) baths. The model has three (meta)stable fixed points (solid dots): the local moment (LM), bosonic fluctuating (B-FL), and fermionic strong-coupling (F-SC) fixed points; the open dots are the critical fixed points F-CR and FB-CR; for details see text. The thick line corresponds to a line of continuous boundary phase transitions. In the metallic case, $r = 0$, the LM and F-CR fixed points merge [1, 2].

$J_K = 0$, the Bose-Kondo model describes an impurity moment in an insulating quantum antiferromagnet [10].

RG analysis. At the bulk quantum critical point we have $\Delta_s = 0$, and both fermionic and bosonic baths obey a power law DOS. The impurity behavior can be analyzed using field-theoretic RG methods, together with an expansion in ϵ and r , similar to Refs. 1, 2, 10.

We employ a pseudo-fermion representation of the impurity spin $\frac{1}{2}$, $\vec{S} = f_\sigma^\dagger \vec{\sigma}_{\sigma\sigma'} f_\sigma$. Following the standard procedure [11], we introduce renormalized fields $f_\sigma = \sqrt{Z_f} f_{R\sigma}$, $\phi_\alpha = \sqrt{Z_\phi} \phi_{R\alpha}$, and dimensionless couplings $K_0 \gamma_0 = \mu^{\epsilon/2} [\tilde{Z}_\gamma / (Z_f \sqrt{Z})] \gamma$, $N_0 J_K = \mu^{-r} (Z_J / Z_f) j$, where μ is a renormalization energy scale. The derivation of the RG equations has been presented in Ref. 2 for non-interacting ϕ bosons ($Z = 1$ in this case). A similar procedure for the present case with a fermionic pseudogap DOS, using the minimal subtraction scheme, gives the following result for the RG beta functions:

$$\begin{aligned} \beta(\gamma) &= -\frac{\epsilon\gamma}{2} + \gamma^3 - \gamma^5 + \frac{j^2\gamma}{2}, \\ \beta(j) &= rj - j^2 + \frac{j^3}{2} + j\gamma^2 - j\gamma^4. \end{aligned} \quad (2)$$

The full two-loop result for the case of interacting bosons will be given elsewhere. The equations (2) reduce to the cases of the pseudogap Kondo model for $\gamma = 0$ [6] and the metallic Bose-Fermi Kondo model for $r = 0$ [2]. Besides the decoupled (local moment – LM) fixed point, $\gamma^* = j^* = 0$, the above flow equations have three non-trivial fixed points which are perturbatively accessible:

B-FL: $\gamma^{*2} = \frac{\epsilon}{2} + \frac{\epsilon^2}{4}$, $j^* = 0$ corresponds to a stable fixed point where the fermionic Kondo coupling is irrelevant, and the coupling between impurity and bosonic bath leads to universal local-moment fluctuations [10];

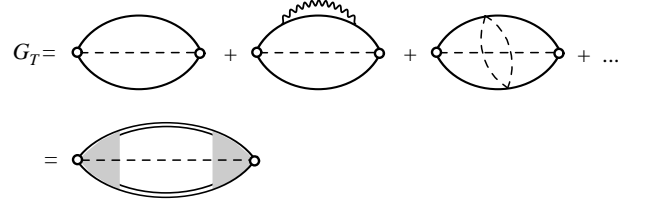


FIG. 2: Feynman diagrams for the Green's function G_T entering the conduction electron T matrix. Full/dashed/wiggly lines denote $f/c/\phi$ propagators. The double line is the full f propagator, the shaded area the full vertex, and the open dots are the external sources.

F-CR: $j^* = r + \frac{r^2}{2}$, $\gamma^* = 0$ is an unstable fixed point controlling the transition between the decoupled (free) moment and the Kondo-screened moment phases; and FB-CR: $\gamma^{*2} = \frac{\epsilon}{2} + \frac{\epsilon^2}{8} - \frac{\epsilon r}{2} - \frac{r^2}{2}$, $j^* = r + \frac{\epsilon}{2}$ – this is an unstable fixed point between the bosonic fluctuating and the Kondo-screened phases.

For large enough j , γ is irrelevant, and the model reduces to the fermionic pseudogap Kondo model which shows strong-coupling phases with screening. Numerical work [8] has shown that, depending on the value of the exponent r and the presence or absence of particle-hole symmetry, two different strong-coupling fixed points exist. As these are not accessible within the present perturbation expansion, we will not distinguish between them, and simply denote the fermionic strong-coupling fixed point, reached for large j and small γ , with F-SC. The flow diagram resulting from this discussion is shown in Fig. 1. In the presence of bosonic interactions the RG flow is similar, and the location of the fixed points is modified only at order ϵ^2 . We expect the general structure of the phase diagram, Fig. 1, to be valid for all ϵ and r values between 0 and 1 – this is e.g. the result of large- N calculations (see below); for $r > \frac{1}{2}$ particle-hole asymmetry is needed to reach the F-SC fixed point. Finally, a finite host spin gap, $\Delta_s > 0$, will cut-off the RG flow of γ at the scale Δ_s , but there is still a transition as function of J_K controlled by the F-CR fixed point.

T matrix. An important quantity is the conduction electron T matrix, describing the scattering of the c electrons off the impurity. It is useful to define a propagator, G_T , of the composite operator $T_\sigma = f_\sigma^\dagger f_{\sigma'} c_{\sigma'}$, such that the T matrix is given by $T(\omega) = J_K^2 G_T(\omega)$. The diagrams for G_T in perturbation theory are shown in Fig. 2. At the RG fixed points, we expect a power law behavior of the T matrix spectral density, with an anomalous exponent η_T . (Note that at tree level $G_T \propto \omega^r$ in the present pseudogap problem.) Within the standard scheme [11] we can obtain the G_T renormalization factor Z_T in an expansion in γ and j by evaluating the lowest-order diagrams and demanding the resulting expression to be free of poles at energy μ . From Z_T we obtain a perturbative expression for η_T according to $\eta_T = \partial(\ln Z_T) / \partial(\ln \mu)$, evaluated at $j = j^*$ and $\gamma = \gamma^*$.

However, it is possible to obtain an *exact* result for η_T , valid to all orders in perturbation theory. The argument parallels the one for anomalous exponent of the local susceptibility in Refs. [2, 10]: Inspecting the diagrams in the upper panel of Fig. 2 shows that all are obtained from the first diagram with *full* j vertices and *full* f electron propagators, i.e., there are no additional processes involving, e.g., the conduction electron line. This gives the relation $Z_T^{-1} = Z_J^2/Z_f^2$ [12]. Using the definition of Z_J and taking the derivative w.r.t. $(\ln \mu)$ at fixed bare J_K , we obtain $0 = -r + \beta(j)/j - \eta_T/2$. Thus, at any RG fixed point with finite, non-zero j^* , we find the exact result

$$\eta_T = -2r \Rightarrow T(\omega) \propto \frac{1}{\omega^{-r-\eta_T}} = \omega^{-r}. \quad (3)$$

This result applies to both critical fixed points (F-CR and FB-CR), and relies only on the fact that the c electrons do not have a self-interaction being relevant in the RG sense, i.e., it holds for interacting ϕ bosons as well.

Remarkably, the critical behavior $T(\omega) \propto \omega^{-r}$ has been numerically found in studies of the pseudogap Kondo model, i.e., at the F-CR fixed point [7, 13]. It is also obtained within a dynamic large- N analysis of the same problem [9].

Application to cuprate superconductors. In superconducting cuprates it is reasonable to separate the low-energy degrees of freedom into Bogoliubov quasiparticles around the nodes of the d -wave superconducting order parameter, and antiferromagnetic spin fluctuations around wavevector $\mathbf{Q} = (\pi, \pi)$, as manifest in the resonance peak in neutron scattering [14]; momentum conservation prohibits a low-energy coupling between fermionic and bosonic degrees of freedom. A phenomenological description of cuprates in terms of a BCS superconductor plus low-energy collective spin excitations [15] has been successful in describing a number of recent neutron scattering and STM experiments. Therefore, impurity moments in cuprate d -wave superconductors can be expected to be well described by the pseudogap Fermi-Bose Kondo model, with fermionic DOS exponent $r=1$.

Experimentally, signatures of Kondo physics have been observed in cuprates doped e.g. with Zn replacing Cu [16, 17] – here the non-magnetic Zn induces a quasi-free magnetic moment in its vicinity, which can be related to the properties of the parent Mott insulator [18]. In particular, NMR experiments indicate Kondo screening of Zn-induced moments in optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ below the superconducting T_c , but show that screening is suppressed in underdoped samples [17]. So far, theoretical analysis has been restricted to either a moment interacting with bulk spin fluctuations [10] or a moment interacting with Bogoliubov quasiparticles [6, 13, 19].

Here we propose that the increasing strength of antiferromagnetic fluctuations is the most important contribution to the T_K suppression in underdoped cuprates. To this end, we calculate the Kondo temperature in the

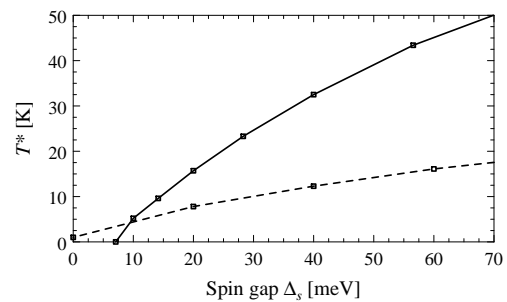


FIG. 3: Characteristic energy scale T^* as function of the bosonic spin gap Δ_s , calculated for a fermionic host corresponding to a cuprate superconductor [13], using large- N techniques. Solid: $J_K = 0.27$ eV, $U = -0.15$ eV, $\gamma_0 = 0.15$ eV; Dash-dot: $J_K = 0.38$ eV, $U = 0$, where U is the additional impurity scattering potential. In comparison with NMR experiments, T^* is equivalent to the Kondo temperature below which the impurity moment is screened; the horizontal axis can roughly be identified with doping (up to $\Delta_s \approx 50$ meV) [14]. Note that the change in the fermionic band upon doping has little influence on T^* ; an increase in the superconducting gap, Δ_0 , with underdoping will further suppress T^* .

pseudogap Fermi-Bose Kondo model for a realistic band structure in H_f and a spin fluctuation spectrum in H_b with varying spin gap Δ_s . In modelling the experiment, the important ingredient is that Δ_s decreases with underdoping, as observed in neutron scattering [14] – from the RG analysis it is clear that decreasing Δ_s can drive the impurity from the F-SC to the LM phase. For H_f we use a standard d -wave BCS model with a gap function $\Delta_{\mathbf{k}} = (\Delta_0/2)(\cos k_x - \cos k_y)$.

To obtain quantitative results, we employ a large- N approach where the spin symmetry is generalized from $SU(2)$ to $SU(N)$. The methodology is similar to earlier work [5, 10, 19, 20], details will be published elsewhere. While this method has artifacts near the quantum-critical points discussed above, and is not quantitatively accurate, we expect it to capture the qualitative low- T physics. The $T = 0$ results allow to extract a low-energy scale, namely the position of the peak in the T matrix, $k_B T^*$, which can be identified with the Kondo temperature up to a numerical factor of order unity [13, 19]. Fig. 3 shows sample results for this quantity as function of the bulk spin gap, Δ_s .

These results indicate that antiferromagnetic fluctuations with a small spin gap Δ_s are effective in suppressing Kondo screening. We note that an increasing superconducting gap, Δ_0 , upon underdoping can have a similar effect in the pseudogap Kondo model [13]. However, this mechanism is less likely to be universal for all cuprates, as a strong doping dependence of Δ_0 has been observed in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ but not in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$. In contrast, spin fluctuations grow upon underdoping in all cuprates. Therefore, we propose the suppression of Kondo screening as observed in NMR [17] to be well explained within the pseudogap Fermi-Bose Kondo model

with a doping-dependent host spin gap.

Application to heavy-fermion metals. Motivated by neutron scattering experiments on the heavy-fermion compound $\text{CeCu}_{6-x}\text{Au}_x$ [4], which indicate momentum-independent critical dynamics at an antiferromagnetic ordering transition, Si *et al.* proposed a self-consistent version of the Fermi-Bose Kondo model as a candidate to describe such critical behavior within an extended dynamical mean-field approach (EDMFT) [3]. In this scenario, the critical point of the lattice model is mapped onto the critical point (BF-CR) of the impurity model.

The self-consistency within EDMFT has to be achieved for both fermionic and bosonic baths. So far, most discussions assumed $r = 0$ and focussed primarily on the bosonic part [2, 3]. Here we want to draw attention to the fermionic part as well. Our analysis above shows that a fermionic bath with $|\omega|^r$ spectrum leads to a impurity T matrix with power-law divergence $|\omega|^{-r}$ (3) at the critical point. Now the question is whether DMFT self-consistency in the fermionic bath of a Kondo or Anderson lattice model can be achieved with such a power law. Consider the DMFT self-consistency relation for an Anderson lattice model, where the T matrix corresponds to $V^2 G_{\text{imp}}$ [5]:

$$G^{\text{loc}}(z) = \int d\epsilon \frac{\rho_0^c(\epsilon)}{z - \epsilon_f - \Sigma^f(z) - \frac{V^2}{z - \epsilon}} \quad (4)$$

$$= [z - \epsilon_f - \Delta(z) - \Sigma^f(z)]^{-1} = G_{\text{imp}}(z)$$

in standard notation, with $\rho_0^c(\epsilon)$ the DOS of the bare conduction band of the lattice model, Σ^f the interacting impurity self-energy, and $\Delta(z)$ the effective hybridization function for the impurity model. Now, $G_{\text{imp}} \propto \omega^{-r}$ implies $\text{Im}[\Delta(\omega) + \Sigma^f(\omega)] \propto -|\omega|^r$. As Σ^f is identified with the lattice self-energy within DMFT, we require $\text{Im}\Sigma^f < 0$, and both $\text{Im}\Delta(\omega)$ and $\text{Im}\Sigma^f(\omega)$ have to vanish as $-|\omega|^r$. Using the ansatz $\Sigma^f(z) = -\epsilon_f + Az^r$ and expanding $\rho_0^c(\epsilon)$ around $\epsilon = 0$, the integral in the first line of (4) can be performed in the limit of small z , and, surprisingly, the coefficient of the leading z^{-r} term in $G^{\text{loc}}(z)$ vanishes.

Therefore, critical-point self-consistency in the fermionic sector of EDMFT for an Kondo or Anderson model *cannot* be achieved with an exponent $r > 0$. If a local critical point within EDMFT exists, it is thus characterized by $r = 0$, and in this case logarithmic corrections in the T matrix are expected, leading to a logarithmic temperature dependence of the resistivity. In addition, we note that any such critical point will be characterized by an extensive ground state entropy

(this holds for arbitrary r), which should have strong signatures in specific heat experiments.

Conclusions. We have analyzed a Fermi-Bose Kondo model, describing an impurity spin coupled to both fermionic quasiparticles with a pseudogap DOS and collective mode bosons, using renormalization group and large- N techniques. We have argued our findings to be relevant for cuprate superconductors as well as for scenarios of local criticality in heavy-fermion metals.

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- [1] J. L. Smith and Q. Si, Europhys. Lett. **45**, 228 (1999); A. M. Sengupta, Phys. Rev. B **61**, 4041 (2000).
 - [2] L. Zhu and Q. Si, Phys. Rev. B **66**, 024426 (2002); G. Zarand and E. Demler, Phys. Rev. B **66**, 024427 (2002).
 - [3] Q. Si, S. Rabello, K. Ingersent, and J. L. Smith, Nature **413**, 804 (2001) and cond-mat/0202414.
 - [4] A. Schröder *et al.*, Nature **407**, 351 (2000).
 - [5] A. C. Hewson, *The Kondo Problem to Heavy Fermions*, Cambridge University Press, Cambridge (1997).
 - [6] D. Withoff and E. Fradkin, Phys. Rev. Lett. **64**, 1835 (1990). C. R. Cassanello and E. Fradkin, Phys. Rev. B **53**, 15079 (1996) and **56**, 11246 (1997).
 - [7] R. Bulla, T. Pruschke, and A. C. Hewson, J. Phys.: Condens. Matter **9**, 10463 (1997), R. Bulla, M. T. Glossop, D. E. Logan, and T. Pruschke, *ibid* **12**, 4899 (2000).
 - [8] C. Gonzalez-Buxton and K. Ingersent, Phys. Rev. B **57**, 14254 (1998); K. Ingersent and Q. Si, Phys. Rev. Lett. **89**, 076403 (2002).
 - [9] M. Vojta, Phys. Rev. Lett. **87**, 097202 (2001).
 - [10] S. Sachdev, C. Buragohain and M. Vojta, Science **286**, 2479 (1999); M. Vojta, C. Buragohain and S. Sachdev, Phys. Rev. B **61**, 15152 (2000).
 - [11] E. Brezin, J.C. Le Guillou, and J. Zinn-Justin, in *Phase transitions and critical phenomena*, eds. C. Domb and M. S. Green, Page Bros., Norwich (1996), Vol. 6.
 - [12] A relation between Z factors can only be formulated for a true propagator like G_T , not for a self energy.
 - [13] M. Vojta and R. Bulla, Phys. Rev. B **65**, 014511 (2002).
 - [14] H. F. Fong *et al.*, Phys. Rev. B **61**, 14773 (2000).
 - [15] E. Demler, S. Sachdev, and Y. Zhang, Phys. Rev. Lett. **87**, 067202 (2001); A. Polkovnikov, M. Vojta, and S. Sachdev, Phys. Rev. B **65**, 220509 (2002).
 - [16] H. Alloul *et al.* Phys. Rev. Lett. **67**, 3140 (1991).
 - [17] J. Bobroff *et al.*, Phys. Rev. Lett. **83**, 4381 (1999) and **86**, 4116 (2001).
 - [18] A. M. Finkelstein *et al.*, Physica C **168**, 370 (1990); S. Sachdev and M. Vojta, cond-mat/0009202.
 - [19] A. Polkovnikov, S. Sachdev, and M. Vojta, Phys. Rev. Lett. **86**, 296 (2001).
 - [20] S. Burdin *et al.*, Phys. Rev. B **67**, 121104 (2003).